THE MANUAL CALCULATION of the quantities of individual amino acids from the charts produced by an automatic amino acid analyzer, especially in complex natural mixtures, can be extremely tedious and time-consuming. To at least partially eliminate these factors, a system has been designed which converts the millivoltage output of the three photocells of an analyzer, built to the specifications of Spackman, Moore, and Stein (*2*), to IBM[b] coded tape. This tape is used as the input for a properly programmed electronic computer. By this means, a complete basic amino acid analysis or a neutral and acidic amino acid analysis can be calculated in from 8 to 16 minutes, depending upon the kind and amount of information sought, with an accuracy equal to or better than that obtained by the manual procedure.

The interest in a system for computer calculation, such as this, is quite widespread as evidenced by the number of inquiries received from those who have heard of it by various means. Although other approaches, somewhat different from the one being described, are known to be under study both in research laboratories (*1*) and probably in instrument companies, this brief description is presented because of its demonstrated practicability.

In the application described, the output signals of the analyzer photometer are in the form of analog signals. However, this is complicated by the use of three photocells the outputs of which must be monitored simultaneously. One represents the amount of 570-mμ light transmitted by the solution, another represents the amount of 440-mμ light transmitted, and the third represents the amount of 570-mμ light transmitted by the same solution but through a shorter path distance than the first. The data collection system must accept each of these analog signals, convert them to digital forms, and record them on punched paper tape in the order given.

In addition, each individual digital data point must be recorded at the identical time its corresponding analog point is being recorded on the analyzer recording chart. This is necessary because two recording potentiometers, when used in parallel, must balance at the same time if accurate values are to be obtained. (Potentiometers tend to draw current until they balance and thus reduce the voltage measured.) Also this allows the operator easily to determine the peak volumes for each amino acid to be used by the computer for identification. Use of the analog chart also allows the operator to determine the success or failure of a run.

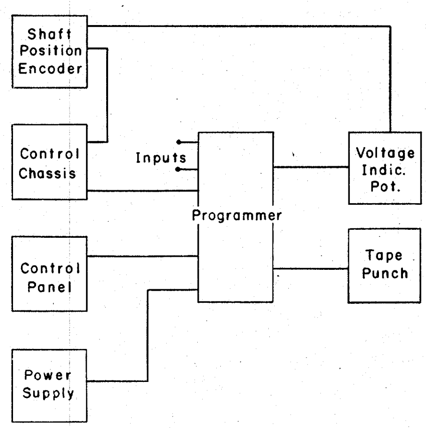

Figure 1. Diagram of analog to digital converter

Simple use requirement specifications were drawn up and submitted for bids by electronic equipment manufacturers. The successful bidder then produced a combination of modules required to fulfill the specifications.

System Description. A block diagram of the analog to digital converter and punch is given in Figure 1.

The voltage indicating potentiometer receives the 0- to 10-mv. analog signal from the amino acid analyzer and rotates the shaft position encoder to a corresponding position. This encoder provides a direct digital output corresponding to the angular position of the indicator shaft. The control chassis stores and translates the digitally coded output of the encoder to decimally coded contact closures. The programmer provides controls to perform system functions according to a prearranged format. The control panel provides circuit breakers for system power, selects operating mode, and controls record and reset functions. The power supply provides the d.c. power and amperage required for operation of the other components. The tape punch punches the paper tape according to the commands received from the programmer.

The above description, although general in nature, provides sufficient information for a manufacturer to build or assemble the components required for this application. However, several accessory items are necessary to relate the digitizer to the automatic analyzer and to make the tape completely compatible with the paper tape reader on the computer.

Accessory Equipment. A three-place stepping switch was mounted on the same shaft as the stepping switch in the analyzer recorder. Only the 570-mμ full light path photocell terminal is connected to the digitizer to give switch closure just prior to the 570-mμ full light path photocell data point. This signal is fed to a counter which records seven data points from this photocell which correspond to 21 data points (63 digits) for the three photocells, and then command the digitizer to punch the end of line code. This is required to orient the computer with respect to the sequence of points if some mechanical or electrical trouble is encountered. This number of data points was chosen because these points can be conveniently read into the computer memory as a unit. Therefore, both tape quantity and computer time are saved.

A tandem microswitch was installed on the analyzer recorder to produce a contact closure when a dot on the chart is being printed. This signals the converter to read the data and punch them into the tape for the reasons discussed above.

The input leads to the converter were connected to the input terminals of the analog recorder amplifier between the amplifier and the recorder stepping switch. In this way the photocells were connected, in turn, to both potentiometers in the same way at the same time. In this case the converter indicating potentiometer has a one-second balance time compared to five seconds for the analyzer multipoint recorder.

The output of the converter is an eight-channel tape which, in this case, is punched in code capable of being read by the tape reader for an IBM 1620 computer. In addition to the digit values (three digits per analog record) in millivolts, a series of tape feed punches (channels 1 through 7) is placed at each end of the digital record to facilitate use with the computer. A switch on the converter is depressed

[a] Eastern Utilization Research and Development Division, Agricultural Research Service, U. S. Department of Agriculture.

[b] Mention of commercial items does not carry its recommendation over any other not mentioned.

for a sufficient length of time to give the required length of tape feed.

In the IBM coding system all digits must have an odd number of holes in the tape. An even number of holes cannot be handled by the computer. A parity checking auxiliary attachment was added to the punch to indicate when an even number of holes was punched due to some difficulty in the converter mechanism so that repair could be accomplished in a minimum of time. This is especially important when considerable time elapses between the tape punching and the actual computer computation.

Sample information, such as column number and sample number, is written on each end of the tape for identification purposes. The computer program requires the effluent volume of each peak and the identification of the amino acid responsible. This information is obtained from the analog record (chart) and is entered in the appropriate place on a line of an 80-column work sheet along with such items as column number, run number, tape start time, total solids, and size of sample. This information is punched from the work sheet into a punch card which is fed into the computer memory to be used when called upon by the computation program.

The electronic computations are made at the U. S. Department of Agriculture Research Service, Biometrics Division, Beltsville, Md. Information about the machine language program can be obtained from that organization if required.

Performance. The instrumentation described has been in use for about 2 years, operating from 5 to 7 days per week. The percentage of lost time due to breakdown of components has been less than 1%. The calculated data have been demonstrated to have an accuracy equal to, or better than, that obtained by the manual calculation from the corresponding analog chart. The higher accuracy results can probably be accounted for through the fact that all data points are employed in the computer calculation of peak areas while only selected points are used in the manual system. Use of this procedure has eliminated the need for one professional chemist per year on the project.

ACKNOWLEDGMENT

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LITERATURE CITED

(1) Moore, S., private communication (1962).

(2) Spackman, D. H., Stein, W. H., Moore, S., ANAL. CHEM. **30**, 1190–1206 (1958).